

Challenges in High Energy Density Physics: Particle Transport and Coupled Physics in the 21st Century

April 19, 2006

Introduction

The purpose of this white paper is to provide a framework for understanding the role that physics and algorithmic issues associated with particle transport are expected to play in successful ASC Predictive Science Academic Alliance Program (PSAAP), and to identify areas of particular interest and relevance to the NNSA Laboratories.

This white paper is closely coupled to the Plasma Physics white paper. Therefore, it is our recommendation that the Particle Transport and Plasma Physics papers be read as a pair. As also stated with regard to the plasma physics topics of interest, the ASC Predictive Science Academic Alliance Program seeks large scale projects that require the successful integration of key physics areas and algorithms into a ‘multi-physics’ framework.

Particle Transport

In a wide variety of applications relevant to high energy density (HED) plasmas, particle motion accounts for a significant fraction of the transport of momentum and energy. Depending on the circumstances, the types of particles might include some combination of photons, charged particles, and neutrons. Typically, the computational time in our simulation programs is dominated by the transport calculation. Therefore, there is a potential for very high leverage progress in formulating and solving transport algorithms in a new manner that reduces the time to solution for many applications.

In current practice, solving the transport equations requires the inversion of a matrix whose size demands the use of implicit (i.e., iterative) methods rather than direct solution; therefore, the biggest gains in computational efficiency are to be made in finding techniques to accelerate convergence. The challenge is that some of these acceleration methods are very application specific because they are physics based; others are very general because they address the mathematics of the transport equation [1].

The numerical simulation of transport is further complicated by the strong nonlinearity of the transport coefficients (e.g., as a function of temperature or density), the coupling with the plasma dynamics and by the large range of time scales involved. Jacobian free Newton-Krylov techniques provide a natural framework for solving nonlinear time implicit equations under these conditions. The efficiency of these methods can be greatly improved by the use of physics-based preconditioners whose development is still in its infancy [2].

Additionally, most multi-physics simulation codes still use operator splitting as a strategy to deal with coupled processes. However, recent work [3] has demonstrated serious problems with operator splitting, especially when the coupled processes have very different time scales. Unfortunately, the solution of the fully coupled nonlinear equations is currently impracticable given the few alternatives to operator splitting that exist at present.

The potential problems of operator splitting raise another numerical issue in the realm of verification and validation of codes. For example, it is possible to conceive of a perfect hydrodynamics algorithm coupled with a perfect radiative transport algorithm, whose operator split combination nevertheless generates large errors. These errors could not be identified through unit testing, implying the need for analytic solutions to complex coupled problems for application as a basis for multi-physics code validation.

Particle Transport in Heterogeneous Materials

The last 20 years has seen an explosion of interest in the theoretical treatments of particle transport in heterogeneous material. In a simulation, it is almost impossible to capture all of the scales of heterogeneity present within a given mesh resolution. Capturing the sub-grid scale material behavior and then determining how it influences particle transport at a coarser level is at the heart of a variety of theoretical treatments [4]. Unfortunately, even with considerable theoretical effort the general problem of particle transport in a participating stochastic medium with a non-Markovian chord length distribution remains unsolved. In addition, when coupled to hydrodynamic motion (e.g., radiation transport in a turbulent medium) the problem becomes extremely complex. Understanding through simulation the behavior of particle transport through non-Markovian participating media with or without hydrodynamic motion would help identify weaknesses in current theoretical models and point in directions where theoretical developments are needed.

Radiation-Hydrodynamics

The consequence of large radiation pressures in hot dense radiative (HDR) plasmas is a tight coupling between hydrodynamic motion of the material and radiative processes. Additionally, Radiation flow in the presence of large hydrodynamic velocity gradients is a well known challenge both computationally and experimentally. The numerical issues faced by transport codes raised above apply here as well, with the added complexity of how to solve the coupled radiation-hydrodynamic equations. As pointed out above, traditional methods rely on an operator splitting technique with its attendant difficulties. Newer methods attempt to solve the full set of equations via Godunov schemes [5]. Is there an advantage going to fully integrated approaches as opposed to operator splitting methods when comparing computational cost for a given level of accuracy? What happens if a third piece of physics is needed?

Furthermore, material motion in the presence of radiation transport presents challenges for mesh strategies. If the mesh is Eulerian, the radiation transport package must be able to deal with material interfaces not aligned with zone boundaries. If the mesh is

Lagrangian, there is the difficulty of representing complex flows with concomitant zonal advection of material dependent transport coefficients. Arbitrary Lagrangian Eulerian (ALE) methods seem to be the choice of many coupled physics codes. However, then it is frequently necessary to propagate the radiation front across highly distorted zones. Are there more accurate and robust spatial discretizations for the diffusion and transport operators? Typically, the hydrodynamics dictates the mesh motion. Should the radiation and hydrodynamics be solved on separate meshes, each best suited to their respective needs?

Radiation-Magneto-Hydrodynamics

Recent advances in pulsed power technology have revived research on fast implosion of annular current sheets known as dynamic Z-pinches. Applications include the generation of x-ray radiation, equation of state measurements, thermonuclear fusion, and more recently the possibility of laboratory based astrophysics experiments analogous to those done with lasers. Simulations of Z-pinches require radiation-magneto-hydrodynamics models. The inclusion of resistive MHD into a radiation-hydrodynamic model introduces a host of plasma instabilities including the magnetic-Raleigh-Taylor instability, as well as the dominant $m=0$ and $m=1$ MHD instabilities. Under some conditions, the Hall term can be appreciable and lead to modification of the plasma evolution. The resistive MHD equations provide a very good approximation to a wide range of the parameters sampled by both liners and wires. As such, most of the macroscopic phenomena are well modeled. On the other hand, details of MRT saturation mechanisms, wire-coronal formation and evolution, liner bubble break-through, and initial MRT seed perturbation wavelengths are probably not well modeled. These physical processes tend to sample plasma parameter regimes which require physics described by two-fluid MHD.

Laser-Plasma Interaction:

Understanding laser-plasma interactions (LPI) is critical to many applications of interest to the NNSA National Laboratories. For example, almost every experimental arena applying laser-plasma phenomena requires an understanding of LPI. A generic challenge has been and continues to be control of the propagation of moderate (10^{15} watts/cm²) to high (10^{20} watts/cm²) intensity light through plasmas at an electron density at or above $\sim 10^{21}$ cm⁻³. The radiation-hydrodynamic codes that are very predictive when the light propagation is well described by geometric optics fail dramatically when collective plasma instabilities affect the propagation. Only in the last decade have the programmatic demands on laser-plasma interaction demanded quantitative design tools that simulate light propagation in high energy density plasmas. The challenge is to develop models that are adequate to describe the non-linearities that govern the evolution of large amplitude plasma waves.

References

- 1) F. Graziani and G. Olson, "Transport Methods: Conquering the Seven Dimensional Mountain", SCaLeS Workshop, UCRL-JC-154432.
- 2) V. Mousseau, D. Knoll, W. Rider, " Physics-based Preconditioning and the Newton-Kryov Method for Non-equilibrium Radiation Diffusion, J. Comp. Phys. **160**, 743 (2000).
- 3) D. Knoll, L. Chacon, L. Margolin, V. Mousseau, "On Balanced Approximations for Time Integration of Multiple Time Scale Systems," J. Comp. Phys. **185**, 583 (2003).
- 4) G. Pomraning, "Linear Kinetic Theory and Particle Transport in Stochastic Mixtures", **World Scientific** (1991).
- 5) Dai and Woodward, J. Comp. Phys. **157**, 199 (2000)..

Points of Contact

Frank Graziani
Lawrence Livermore National Laboratory
graziani1@llnl.gov

Len Margolin
Los Alamos National Laboratory
len@lanl.gov

Thomas Mehlhorn
Sandia National laboratories
tamehlh@sandia.gov

Acknowledgements

The authors wish to thank the help and contributions of many colleagues. In particular, Brian Albright, Denise Hinkel, Dana Knoll, Bruce Langdon, and Dan Winske deserve special thanks for their contributions.

This work was, in part, performed by the Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratories under auspices of the U.S. Department of Energy.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.